Electric Multipole Moments for Some First-Row Diatomic Hydride Molecules

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Abstract: As an example of the use of the analytical formulas derived for electric multipole moment integrals over STOs in our previous work (I.I. Guseinov, et al., J. Mol. Struct. (Theochem) 465 (1999) 5), the 2^ν-pole electric moments have been calculated for the ground electronic states of LiH, BH and FH of the first-row diatomic hydride molecules. Calculated electric multipole moment values are in agreement with literatures. By the use of these analytical formulas the 2^ν-pole moments for multiatomic molecules can be evaluated most efficiently and accurately by employing STOs as basis sets.

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